=> s 11

SAMPLE SEARCH INITIATED 11:59:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 96966 TO ITERATE

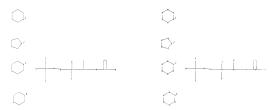
2.1% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*
PROJECTED ITERATIONS: 1920831 TO 1957809
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=>

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chain nodes :

1 2 3 4 5 6 7 8 9 11 12 13 15 44

16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38

ring/chain nodes :

14

chain bonds :

1-11 1-9 1-8 1-44 2-3 2-11 3-4 3-12 3-13 4-5 4-14 5-6 6-7 6-15

G1:C,O,N

G2:[\*1],[\*2],[\*3],[\*4]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 26:Atom 27:Atom 28:Atom 30:Atom 31:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 36:Atom 37:Atom 38:Atom 36:Atom 37:Atom 37:Atom 38:Atom 37:Atom 37:Atom 38:Atom 37:Atom 37:Atom 38:Atom 37:Atom 37:Atom 37:Atom 38:Atom 37:Atom 38:Atom 37:Atom 37:Atom 38:Atom 38

0 ANSWERS

Generic attributes :

15:

Saturation : Unsaturated

#### L3 STRUCTURE UPLOADED

=> s 13

SAMPLE SEARCH INITIATED 12:07:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 43107 TO ITERATE

4.6% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 849741 TO 874539

0 TO 0

PROJECTED ANSWERS:

L4 0 SEA SSS SAM L3

=> s 13 sss full FULL SEARCH INITIATED 12:07:14 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 862126 TO ITERATE

95.8% PROCESSED 825571 ITERATIONS 84 ANSWERS

100.0% PROCESSED 862126 ITERATIONS 86 ANSWERS SEARCH TIME: 00.00.24

SEARCH 11ME: 00.00.24

L5 86 SEA SSS FUL L3

=> file caplus COST IN U.S. DOLLARS FULL ESTIMATED COST

SINCE FILE 178.40

TOTAL. ENTRY SESSION 178.61

FILE 'CAPLUS' ENTERED AT 12:07:46 ON 27 DEC 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 27 Dec 2007 VOL 147 ISS 26 FILE LAST UPDATED: 26 Dec 2007 (20071226/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s 15

22 L5 L6

=> d 16 1-22 bib abs hitstr

- L6 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2007:705111 CAPLUS
- DN 147:143660
  - Preparation of 3-chloro-4-isopropoxybenzamide and 3-cyano-4-
  - isopropoxybenzamide derivatives as inhibitors of mitotic kinesins
- Oian, Xiangping; Ashcraft, Luke W.; Wang, Jianchao; Yao, Bing; Jiang, Hong; Bergnes, Gustave; Morgan, Bradley P.; Morgans, David J.; Dhanak, Dashyant; Knight, Steven D.; Adams, Nicholas D.; Parrish, Cynthia A.; Duffy, Kevin J.; Fitch, Duke; Tedesco, Rosanna
- PA IISA SO
- U.S. Pat. Appl. Publ., 171pp., Cont.-in-part of U.S. Ser. No. 271,147. CODEN: USXXCO
- DT Patent LA English

F	AN.CN		TENT NO.	KIND	DATE	AP	PLICATION NO.	DATE	DATE		
P	T 1	10	2007149516	A1	20070628	110	2006-598250	20061108			
E			2007143316	A1	20070028		2005-271147	20051108			
ъ			2005-271147	A2	20051102	0.0	2003 271147	20031103			
-			2003-271147 2004-569510P	P	20031103						
			2005-121709	A2	20050503						
			2005-124608	A2	20050506						

R2

Ι

AB The title compds. [I; R1 = 3-halo-4-((R)-1,1,1-trifluoropropan-2vloxy) phenyl, 3-cvano-4-((R)-1,1,1-trifluoropropan-2-vloxy) phenyl, 3-halo-4-isopropylaminophenyl, 3-cyano-4-isopropylaminophenyl, 3-halo-4-((R)-1,1,1-trifluoropropan-2-ylamino)phenyl, 3-cyano-4-((R)-1,1,1trifluoropropan-2-ylamino)phenyl; X = CO, SO2; R2 = H, (un)substituted lower alkyl; W = CR4, CH2CR4, N; R3 = COR7, H, each (un)substituted substituted alkyl, heterocycloalkyl, heteroaryl, or aryl, cyano, sulfonyl; R4 = H, (un)substituted alkyl; R5 = H, HO, each (un)substituted amino, cycloalkyl, heterocycloalkyl, heteroaryl, or lower alkyl; R6 = H, CONH2, (un) substituted alkyl, alkoxy, aryloxy, heteroaryloxy, alkoxycarbonyl, aryl, heteroaryl, cycloalkyl, or heterocycloalkyl; R7 = HO, each (un) substituted lower alkyl, aryl, amino, aralkoxy, or alkoxy; provided that if W is N, then R5 is not hydroxy or (un)substituted amino, and R6 is not optionally substituted alkoxy, optionally substituted aralkoxy, optionally substituted heteroaralkoxy, or optionally substituted amino] are prepared (1R)-1-(methoxycarbonylamino)-1-[4-[4-[(2S)-2-[[[4-(((1R)-2,2,2-trifluoroisopropyl)oxy)-3-chlorophenyl]carbonyl]amino]-4hydroxybutyl]phenyl]-1-ethylimidazol-2-yl]ethane. These compds. including N-benzoyl-amino alcs., N-benzoyl-amino acid amide, N-benzoylsemicarbazide, and N-benzovl-diamine derivs. are inhibitors of one or more mitotic kinesins and are useful in the treatment of cellular proliferative diseases, for example cancer, hyperplasias, restenosis, cardiac hypertrophy, immune disorders, fungal disorders, and inflammation by modulating the activity of one or more mitotic kinesins. Thus, cyclocondensation of (2S)-2-(tert-butoxycarbonylamino)-5-bromo-4oxopentanoic acid Me ester with thiobenzamide in the presence of diisopropylethylamine in methanol under refluxing for 24 h gave (2S)-2-(tert-butoxycarbonylamino)-3-(2-phenylthiazol-4-yl)propanoic acid which was treated with CF3CO2H in CH2Cl2 at room temperature for 10 min to give (2S)-2-amino-3-(2-phenylthiazol-4-yl)propanoic acid (II). II was condensed with 3-chloro-4-isopropoxybenzoic acid pentafluorophenyl ester in the presence of disopropylethylamine in DMF at room temperature to give (2S)-N-methyl-2-[(3-chloro-4-isopropoxybenzoyl)amino]-3-(2-phenylthiazol-4yl)propanamide (III). Many of the compds. I showed GI50 (50% growth inhibition concentration) of ≤10 µM against human ovarian tumor cells Skov-3.

IT 943297-47-0P, N-[(2S)-2-[[[3-Chloro-4-(1methylethoxy)phenyl]carbonyl]amino[-3-[4-[8-(1-hydroxyethyl)-4-

hydroimidazo[1,2-a]pyridin-2-y1]pheny1]propy1]-2-(pyrrolidin-1vl)acetamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-benzoyl amino alcs., N-benzoyl-amino acid, N-benzovlsemicarbazide derivs. as inhibitors of mitotic kinesins) 943297-47-0 CAPLUS

CN 1-Pyrrolidineacetamide, N-[(2S)-2-[[3-chloro-4-(1methylethoxy)benzoyl]amino]-3-[4-[8-(1-hydroxyethyl)imidazo[1,2-a]pyridin-2-y1]phenyl]propyl]- (CA INDEX NAME)

#### Absolute stereochemistry.

- L6 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2004:863107 CAPLUS
- DN 142:48476
- TΙ Nocathiacin I analogues: synthesis, in vitro and in vivo biological activity of novel semi-synthetic thiazolyl peptide antibiotics
- AII Naidu, B. Narasimhulu; Sorenson, Margaret E.; Zhang, Yunhui; Kim, Oak K.; Matiskella, John D.; Wichtowski, John A.; Connolly, Timothy P.; Li, Wenving; Lam, Kin S.; Bronson, Joanne J.; Pucci, Michael J.; Clark, Junius M.; Ueda, Yasutsugu
- CS The Bristol-Myers Squibb Pharmaceutical Research Institute, Wallingford, CT, 06492, USA
- so Bioorganic & Medicinal Chemistry Letters (2004), 14(22), 5573-5577 CODEN: BMCLE8; ISSN: 0960-894X
- Elsevier B.V. PB DT
- Journal
- LA English
- CASREACT 142:48476 os
- Several nocathiacin I analogs were synthesized and evaluated for their AB antibacterial activity. Most of these semi-synthetic analogs retained very good in vitro and in vivo antibacterial activity of nocathiacin I. 807342-65-0P 807342-68-3P
- RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and in vitro and in vivo biol. activity of novel semi-synthetic thiazolyl peptide antibiotics nocathiacin I analogs in relation to aqueous solubility)

RN 807342-65-0 CAPLUS
CN 4-Thiazolecarboxamide, N-[2-amino-1-[[[2-(4-methyl-1-

4-Thiazolecarboxamide, N-[2-amino-1-[[[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-2-(oxtehyl)-2-(18,14E,218,22S,33S,49S)-9,10,11,12,13,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11-[(1R)-1-hydroxyethyl)-14-(1-methoxyethylidene)-9,12,19,30,40,48-hexaoxo-49-[[2,4,6-trideoxy-4-(dimethylamino)-3-C-methyl-ar-1-lyxo-hexopyranosyl]oxy]-22,25-(ethanoxymethano)-8,5:18,15:37,34-trinitrilo-21,33-([2,4]-endo-thiazolomethanimino)-8,15:18,15;37,34-trinitrilo-pyrido[3',2':20,21][1,28,8,18,24,4,11,14]dioxatrithiatriazacyclodotriacontino[30,31-b]indol-2-yll-[9C1] (CA INDEX NAME)

PAGE 1-A

PAGE 3-A

PAGE 4-A

RN 807342-68-3 CAPLUS

CN 4-Thiazolecarboxamide, N-[2-amino-1-[[methyl]2-(1piperidinyl)sthyl]amino]methyl]-2-coxethyl]-2-[(115,14E,21S,22S,33S,49S)9,10,11,12,13,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11[(18)-1-hydroxyethyl]-14-(1-methoxyethyl1dene)-9,12,19,30,40,48-hexaoxo-49[[2,4,6-trideoxy-4-d(dimethylamino)-3-C-methyl-a-L-lyxohexopyranosyl]oxy]-22,25-(ethanoxymethano)-9,5:18,15:37,34-trinitrilo21,33-([2,4]-endo-thiazolomethanimino)-5H,15H,24H,34Hpyrido[3',2':20,21][1,28,8,18,24,4,11,14]dioxatrithiatriazacyclodotriacont
ino[30,31-b]indol-2-v1]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

PAGE 3-A

# RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2004:830103 CAPLUS
- DN 142:1066
- TI Centrally Acting and Metabolically Stable Thyrotropin-Releasing Hormone Analogues by Replacement of Histidine with Substituted Pyridinium
- AU Prokai, Laszlo; Prokai-Tatrai, Katalin; Zharikova, Alevtina D.; Nguyen, Vien; Perjesi, Pal; Stevens, Stanley M., Jr.
- CS Department of Medicinal Chemistry, University of Florida, Gainesville, FL, 32610, USA
- SO Journal of Medicinal Chemistry (2004), 47(24), 6025-6033 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
- LA English

OS CASREACT 142:1066

Metabolically stable and centrally acting TSH-releasing hormone (TRH) AB analogs were designed by replacing the central histidine with substituted pyridinium moieties. Their analeptic and acetylcholine-releasing actions were evaluated to assess their potency as central nervous system (CNS) agents. A strong exptl. connection between these two CNS-mediated actions of the TRH analogs was obtained in subject animals. The analog  $3-(aminocarbony1)-1-(3-[2-(aminocarbony1)pyrrolidin-1-y1]-3-oxo-2-{[(5$ oxopyrrolidin-2-yl)carbonyl]amino}propyl)pyridinium (1a) showed the highest (TRH-equivalent) potency and longest, dose-dependent duration of action from a series of homologous compds. in antagonizing pentobarbital-induced narcosis when administered i.v. in its CNS-permeable prodrug form (2a) obtained via reduction of the pyridinium moiety to the nonionic dihydropyridine. The maximum change in hippocampal acetylcholine concentration upon perfusion of the pyridinium-containing tripeptides into the hippocampus of rats was also achieved with la. No binding to the endocrine TRH receptor was measured for the TRH analogs reported here; therefore, our design afforded a novel lead for centrally acting TRH analogs. We have also demonstrated the benefits of the prodrug approach on the pharmacokinetics and brain uptake/retention of pyridinium-containing TRH analogs (measured by in vivo microdialysis sampling) upon systemic administration.

IT 797054-98-9P

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PRBP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of centrally acting and metabolically stable TSH-releasing hormone analogs by replacement of histidine with substituted pyridinium)

RN 797054-98-9 CAPLUS

CN L-Prolinamide, 5-oxo-L-prolyl-6-[3-(aminocarbonyl)pyridinio]-L-norleucyl-, salt with trifluoroacetic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 738575-25-2 CMF C22 H31 N6 O5

Absolute stereochemistry.

CM

CRN 14477-72-6 CMF C2 F3 O2

#### THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 47 ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
- 2004:610055 CAPLUS AN
- DN 141:157473
- ΤI Preparation of amino acid derivatives as antibacterial agents
- IN Anderson, Neils H.; Bowman, Jason; Erwin, Alice; Harwood, Eric; Kline, Toni; Mdluli, Khisimuzi; Ng, Simon; Pfister, Keith B.; Shawar, Ribhi; Wagman, Allan; Yabannavar, Asha
- PA Chiron Corporation, USA SO
- PCT Int. Appl., 324 pp. CODEN: PIXXD2
- DT Patent
- T.A English

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	PA:	TENT	NO.			KIN	D	DATE			APPL	ICAT	ION	NO.		D.	ATE	
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PI			0626			A2		2004			WO 2	004-	US43	3		2	0040	108
	WO 2004062601					A3		20050421										
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			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,

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    AII 2004204760
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                         A1
                                                                  20040108
    US 2004229955
                         A1
                               20041118
                                           US 2004-754928
                                                                  20040108
    EP 1618087
                         A2
                               20060125
                                           EP 2004-700887
                                                                  20040108
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    CN 1777577
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                                           MX 2005-PA7394
                                                                  20050707
    IN 2005KN01343
                         Α
                               20060915
                                           IN 2005-KN1343
                                                                  20050712
    US 2006154988
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PRAI US 2003-438523P
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                               20030108
    US 2003-466974P
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                               20030430
    US 2003-520211P
                         P
                               20031113
    US 2004-754928
                         A1
                               20040108
    WO 2004-US433
                               20040108
    MARPAT 141:157473
OS
GI
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AB Title compds. I [E = absent or H, (un)substituted-alkyl, -alkenyl, -aryl, etc.; L = absent or CONH, NHCO, (un) substituted alkyl, etc.; D = absent or (un) substituted-cycloalkyl, -aryl, -heterocyclyl or -heteroaryl; G = absent or alkene, alkyne, CO, etc.; Y = (un)substituted-cycloalkyl, -aryl, -heterocyclyl or -heteroaryl; X = CO, alkylcarbonyl, alkenylcarbonyl, alkynylcarbonyl, methylene, or when B is absent X and A together form heterocyclic ring; B = absent or substituted aminoalkylcarbonyl; R3 = H or (un) substituted alkyl, or R3 and A together form a cycloalkyl or heterocyclic ring; R4 = H or (un)substituted alkyl, or R4 and A together form a heterocyclic ring; n=0-2; A=H, acetylene, alkyl, etc.; Q= absent or substituted amide, SH, SO2NH2, CO2H, etc.] are disclosed: As well as stereoisomers, pharmaceutically acceptable salts, esters, and prodrugs thereof; pharmaceutical compns. comprising such compds.; methods of treating bacterial infections by the administration of such compds.; and processes for the preparation of the compds. Thus, e.g., II was prepared via

amidation of 3-bromo-4-fluorobenzoic acid with L-threonine Me ester hydrochloride followed by substitution with hydroxylamine hydrochloride. This invention pertains generally to treating infections caused by gram-neg. bacteria. More specifically, the invention described pertains to treating gram-neg infections by inhibiting activity of UDP-3-O-(R-3-hydroxydecanoyl)-N-acetylglucosamine deacetylase (LpxC). Many of I displayed an IC50 value of less than 10  $\mu\text{M}$  with respect to inhibition of LoxC.

IT 728872-42-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of amino acid derivs. as antibacterial agents)
RN 728872-42-2 CAPLUS
CN 1-Pinerarinacestamide, N-[(2S)-2-(hydroxyamino)-3-oxo-2-[[4-

N 1-Piperazineacetamide, N-[(2S)-3-(hydroxyamino)-3-oxo-2-[[4-(phenylethynyl)benzoyl]amino]propyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2004:589539 CAPLUS

DN 141:123573

TI Preparation of (hetero)arvlcarboxamides as factor Xa inhibitors

IN Liebeschuetz, John Walter; Sheehan, Scott Martin; Watson, Brian Morgan

PA Eli Lilly and Company, USA

SO PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DT Patent

LA English

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PAN.	CNII																
	PATENT	NO.			KIN	D	DATE			APPL	ICAT	ION :	NO.		D	ATE	
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PI	I WO 2004060872				A1 2004072			0722	WO 2003-US39101						20031222		
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							MA,										
							RO,									ΤJ,	TM,
							UG,										
	RW:						MW,										
							ТJ,										
		ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,

TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG AU 2003296393 A1 20040729 AU 2003-296393 20031222 EP 1581493 20051005 EP 2003-814680 A1 20031222 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK US 2006052606 A1 20060309 US 2005-539372 PRAI US 2002-436625P Ρ 20021230 WO 2003-US39101 20031222 W OS MARPAT 141:123573 GΙ

- AB Compds. of formula I [Rl = pyrrolidinyl, (substituted) piperidinyl, (substituted) piperazinyl; R2 = (substituted) Ph, indolyl or benzothiophenyl; R3 = (substituted) Ph, pyridyl, furyl, naphthyl, cycloalkyl, alkyl, etc.; Z = CH2, O, (substituted) NH; n = 1-3] are prepared as inhibitors of the serine protease Factor Xa and are useful in the treatment of thrombotic disorders. Thus, II was prepared in several steps. The prepared compds. had Kass values > 1 x 106 L/mol in the enzyme inhibition assay.
- IT 724463-08-99 72463-09-69 724463-10-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
- (preparation of (hetero)arylcarboxamides as factor Xa inhibitors) RN 724463-08-5 CAPLUS
- CN 1H-Indole-6-carboxamide, 3-chloro-N-[(1R)-1-phenyl-2-[2-(4-piperidinyl)ethoxy]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### ●x HC1

RN 724463-09-6 CAPLUS

CN 1H-Indole-6-carboxamide, 3-chloro-N-[(1R)-2-[2-(1-methyl-4-piperidinyl)ethoxy]-1-phenylethyl]-, hydrochloride (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

### ●x HCl

RN 724463-10-9 CAPLUS

CN 1H-Indole-6-carboxamide, 3-chloro-N-[(1R)-1-phenyl-2-[3-(4-piperidinyl)propoxy]ethyl]- (CA INDEX NAME)

#### Absolute stereochemistry.

- IT 724463-63-2P
   RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
  (Reactant or reagent)
- (preparation of (hetero)arylcarboxamides as factor Xa inhibitors)
- RN 724463-63-2 CAPLUS
- CN 1-Piperidinecarboxylic acid, 4-[2-[(2R)-2-[[(3-chloro-1H-indol-6-yl)carbonyl]amino]-2-phenylethoxy]ethyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

#### Absolute stereochemistry.

L6 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN AN

2004:308415 CAPLUS

DN 140:321240

ΤI Preparation of lactam-containing diaminoalkanes, β-amino acids, α-amino acids and derivatives thereof as factor Xa inhibitors

IN Oiao, Jennifer X.; Han, Wei

PA Bristol-Myers Squibb Company, USA

SO PCT Int. Appl., 172 pp. CODEN: PIXXD2

DT Patient.

LA English

FAN.CNT 1

DATE APPLICATION NO. PATENT NO. KIND DATE PΙ WO 2004031145 A2 20040415 WO 2003-US31079 20031001 A3 WO 2004031145 20040701 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG US 2004077635 A1 20040422 US 2003-677063 20031001 AU 2003279735 Α1 20040423 AU 2003-279735 20031001 EP 1558606 20050803 EP 2003-773077 A2 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK 20070607 US 2007-622484 US 2007129361 A1 20070112 P PRAI US 2002-415366P 20021002 P US 2002-417208P 20021009 US 2003-677063 A1 20031001 WO 2003-US31079 W 20031001 MARPAT 140:321240 OS

GI

The title compds. PMM1 [I; one of P and M1 = G and the other -AB; G = II, III (wherein ring D, including the two carbon atoms of ring E to which it is attached, is (un)substituted 5-6 membered ring consisting of carbon atoms and 0-3 heteroatoms selected from N, O, S(O)0-2; ring D may contain 0-3 ring double bonds; ring E = (un)substituted Ph, pyridyl, pyrimidinyl, etc.; alternatively, ring D is absent); M = (un)substituted 3-8 membered linear chain consisting of carbon atoms, carbonyl groups, thiocarbonyl, heteroatoms, and there are 0-2 double bonds and 0-1 triple bond; A = (un) substituted carbocycle, 5-12 membered heterocycle; B = IV (wherein Q1 = CO, SO2; ring Q = (un)substituted 4-8 membered monocyclic or bicyclic ring optionally containing optionally heteroatoms, and optionally fused, etc.; X = absent, CO, SO, SO2, etc.)], useful as inhibitors of trypsin-like serine proteases, specifically factor Xa for treating thromboembolic disorder, were prepared E.g., a 3-step synthesis of V, starting from 1-(4-aminophenyl)-1H-pyridin-2-one and Boc-DL-PHG-OH, was given. The number of compds. I were found to exhibit Ki's of ≤ 10 µM against human factor Xa. The pharmaceutical composition comprising the compound I is

claimed. IT 678175-26-3P 678175-27-4P 678175-33-2P

78175-26-3P 678175-27-4P 678175-33-2P 678175-64-9P 678175-65-0P 678175-70-7P

678176-04-0P 678176-05-1P 678176-10-8P

678176-56-2P 678176-57-3P 678176-62-0P

678176-96-0P 678177-12-3P 678177-13-4P 678177-25-8P 678177-41-8P 678177-42-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of lactam-containing diaminoalkanes,  $\beta$ -amino acids,  $\alpha$ -amino acids and derivs. thereof as factor Xa inhibitors for treating thromboembolic disorder)

RN 678175-26-3 CAPLUS

CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)-(CA INDEX NAME)

RN 678175-27-4 CAPLUS
CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)-(CA INDEX NAME)

RN 678175-33-2 CAPLUS

CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[2-(4-methyl-1piperazinyl)ethoxy]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)- (CA
INDEX NAME)

RN 678175-64-9 CAPLUS CN Benzamide, N-[3-[(5:

EN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)-(CA INDEX NAME)

RN 678175-65-0 CAPLUS

CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)-(CA INDEX NAME)

RN 678175-70-7 CAPLUS

CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[2-(4-methyl-1piperazinyl)ethoxy]methyl]-3-oxopropyl]-4-(2-oxo-1(2H)-pyridinyl)- (CA
INDEX NAME)

RN 678176-04-0 CAPLUS

RN 678176-05-1 CAPLUS

CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[methyl[2-(4-methyl-1piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA
INDEX NAME)

RN 678176-10-8 CAPLUS

CN Benzamide, N-[3-[(4-chlorophenyl)amino]-1-[[2-(4-methyl-1-piperazinyl)ethoxy]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA INDEX NAME)

RN 678176-56-2 CAPLUS CN Benzamide, N-13-1(5-

CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA INDEX NAME)

RN 678176-57-3 CAPLUS

CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[methyl[2-(4-methyl-1piperazinyl)ethyl]amino]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA INDEX NAME)

RN 678176-62-0 CAPLUS

CN Benzamide, N-[3-[(5-chloro-2-pyridinyl)amino]-1-[[2-(4-methyl-1piperazinyl)ethoxy]methyl]-3-oxopropyl]-4-(2-oxo-1-piperidinyl)- (CA
INDEX NAME)

RN 678176-96-0 CAPLUS

CN 2-Thiophenecarboxamide, 5-chloro-N-[3-[2-(2-oxo-1-piperidinyl)ethoxy]-2-[[4-(2-oxo-1(2H)-pyridinyl)benzoyl]amino]propyl]- (CA INDEX NAME)

RN 678177-12-3 CAPLUS

CN 2-Thiophenecarboxamide, 5-chloro-N-[1-[2-(4-methyl-1piperazinyl)ethoxy|methyl]-2-[[4-(2-oxo-1(2H)pyridinyl)benzoyl]amino]ethyl]- (CA INDEX NAME)

RN 678177-13-4 CAPLUS

2-Thiophenecarboxamide, 5-chloro-N-[1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-2-[[4-(2-oxo-1(2H)-pyridinyl)benzoyl]amino]ethyl]- (CA INDEX NAME)

CN

RN 678177-25-8 CAPLUS

CN 2-Thiophenecarboxamide, 5-chloro-N-[2-[[4-(2-oxo-1-piperidinyl)benzoyl]amino]-3-[2-(2-oxo-1-piperidinyl)ethoxy]propyl]- (CA INDEX NAME)

RN 678177-41-8 CAPLUS

CN 2-Thiophenecarboxamide, 5-chloro-N-[1-[[2-(4-methyl-1-piperazinyl)ethoxy]methyl]-2-[[4-(2-oxo-1-piperidinyl)benzoyl]amino]ethyl]-(CA INDEX NAME)

- RN 678177-42-9 CAPLUS
- CN 2-Thiophenecarboxamide, 5-chloro-N-[1-[[methyl[2-(4-methyl-1-piperazinyl)ethyl]amino]methyl]-2-[[4-(2-oxo-1-piperidinyl)benzoyl]amino]ethyl]- (CA INDEX NAME)

- L6 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2004:182658 CAPLUS
- DN 140:235738
- TI Preparation of pyrazolopyrimidines as calcium receptor modulators
- IN Yasuma, Tsuneo; Mori, Akira; Kawase, Masahiro; Kimura, Hiroyuki; Yoshida, Masato; Gyorkos, Albert Charles; Pratt, Scott Alan; Corrette, Christopher Peter

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PA
    Takeda Chemical Industries, Ltd., Japan; Takeda Pharmaceutical Company
    Limited
SO
    PCT Int. Appl., 460 pp.
    CODEN: PIXXD2
    Patient.
LA
    English
FAN.CNT 1
                        KIND DATE APPLICATION NO. DATE
    PATENT NO.
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                                           ______
    WO 2004017908 A2 20040304 WO 2003-US26317 WO 2004017908 A3 20060105
                                                                   20030821
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR,
             TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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20040311 20050914

20040304 CA 2003-2494700 20030821 20040311 AU 2003-265585 20030821 20050914 EP 2003-793273 20030821

20030821

20030821 20050222 20050225 20050315

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK JP 2006510582 T 20060330 JP 2004-529835 20030821 20060510 CN 2003-823938 CN 1771231 A RR 2003013880 A 20071106 BR 2003-13880
US 2006079536 A1 20060413 US 2005-525158
IN 2005KN00280 A 20060418 IN 2005-KN280
NO 200501328 A 20050315 NO 2005-KN280
PRAI US 2002-406012P P 20020826
US 2003-466129P P 20030428
WO 2003-US26317 W 20030821 os MARPAT 140:235738

A1 A1

A2

CA 2494700

EP 1572113

AU 2003265585

- AB The title compds. [I; ring A = (un)substituted 5-7 membered ring; ring B = (un) substituted 5-7 membered heterocyclic ring; X1 = (un) substituted CH, CH2, N or NH; X2 = N or (un) substituted NH; Y = C, (un) substituted CH or N; Z = (un)substituted CH, CH2, N or NH; Ar = (un)substituted cyclic group; R = H, (un)substituted alkyl, etc.; and their salts], useful as calcium receptor modulators, were provided. The compds. II, III [wherein ring A = (un)substituted 5-7 membered ring; Q = C, CR5 (R5 = H, alkyl, hydroxyalkyl, etc.), or N; X1 = CR1 (R1 = H, alkyl, hydroxyalkyl, etc.), CR1R2 (R1 as above; R2 = H, heterocyclyl, etc.); R3 = H, alkyl, hydroxyalkyl, aminoalkyl, etc.; Y = C, CR4 (R4 = H, alkyl, hydroxyalkyl, etc.), or N; R8-R12 = H, (un)substituted alkyl, etc.; X3 = a bond, O, (un)oxidized S, N, (un)substituted NH, C1-2 alkylene; or their salts], were also provided. Thus, reacting amidation of the acid IV [R = H] with 4-(F3C)C6H4C(Et)2NH2 afforded 31% IV [R = 4-(F3C)C6H4C(Et)2NH]. Biol. data were given for selected compds. The pharmaceutical composition comprising the compound I is claimed.
  - II 667922-27-2P RL: PRC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Usea)
- (preparation of pyrazolopyrimidines as calcium receptor modulators)  ${\tt RN} \quad \, 667922-27-2 \quad {\tt CAPLUS}$
- CN Pyrazolo[1,5-a]pyrimidine-3-carboxamide, N-[1,1-dimethyl-2-[[2-(1-piperidinyl)ethyl]amino]ethyl]-4,5,6,7-tetrahydro-5-phenyl-7-(trifluoromethyl)-, (5R,75)-rel- (CA INDEX NAME)

Relative stereochemistry.

L6 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:543696 CAPLUS

DN 137:353286

TI Design, synthesis, and biological evaluation of novel, centrally-acting thyrotropin-releasing hormone analogs

AU Prokai-Tatrai, Katalin; Perjesi, Pal; Zharikova, Alevtina D.; Li, Xiaoxu; Prokai, Laszlo

CS College of Pharmacy, Center for Drug Discovery, University of Florida, Gainesville, FL, 32610-0497, USA

SO Bioorganic & Medicinal Chemistry Letters (2002), 12(16), 2171-2174 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 137:353286 GI

AB Novel, metabolically stable and centrally acting TRH analogs with substituted pyridinium moieties replacing the [Hie2] residue of the endogenous peptide were prepared by solid-phase Zincke reaction. The 1,4-dihydropyridine prodrugs of these analogs obtained after reducing the pyridinium moiety were able to reach the brain and maintain a sustained concentration of the charged, degradation-resistant analogs formed after enzymic

oxidation of the prodrug, as manifested by the analeptic action measured in mice. Among the four analogs reported, compound I showed the highest potency and longest duration of action in reducing the pentobarbital-induced sleeping time compared to the parent TRH. No binding to the endocrine TRH-receptor was measured for I; thus, this

compound emerged as a potent, centrally acting TRH analog.

IT 474520-12-2P

RL: ANT (Analyte); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(solid-phase synthesis, analeptic action, and receptor binding of TSH-releasing hormone pyridine and dihydropyridine analogs)

RN 474520-12-2 CAPLUS

CN L-Prolinamide, 5-oxo-L-proly1-6-[3-(aminocarbonyl)pyridinio]-L-norleucyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● C1-

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2002:247283 CAPLUS

DN 137:6366

TI A Solid-Phase Synthetic Route to Unnatural Amino Acids with Diverse Side-Chain Substitutions

AU Scott, William L.; O'Donnell, Martin J.; Delgado, Francisca; Alsina, Jordi CS Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285. USA

SO Journal of Organic Chemistry (2002), 67(9), 2960-2969

CODEN: JOCEAH; ISSN: 0022-3263 PB American Chemical Society

DT Journal

LA English

OS CASREACT 137:6366

AB Reacting imine derivs. of resin-bound amino acids (i.e.,

3,4-dichlorobenzaldehyde Schiff bases of Wang resin-bound Ala or Phe) with  $\alpha, \varpi$ -dihaloalkanes provides highly versatile intermediates to racemic  $\alpha, \alpha$ -disubstituted amino acids with a wide variety of

side-chain functionality. Two strategies were developed to convert the intermediate m-chloro or m-bromo derivs. to the desired products. Together, they allow the creation of amino acids with diverse functionalities (m-chlorides, nitriles, azides, acetates, thioacetates, thioethers, secondary and tertiary aliphatic amines, and anilines) placed at varying chain lengths (2-5) from the  $\alpha$ -center of

the amino acid. 433220-56-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of side-chain substituted amino acids by alkylating Schiff bases of Phe- or Ala-Wang resins with dihaloalkanes followed by nucleophilic substitutions)

RN 433220-56-5 CAPLUS

CN 1-Pyrrolidinehexanoic acid, α-methyl-α-[(2naphthalenylcarbonyl)amino]- (CA INDEX NAME)

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN 1.6

AN 2002:142742 CAPLUS

DN 136:200481

ΤI Preparation of water-soluble thiazolyl peptide derivatives

IN Naidu, B. Narasimhulu; Li, Wenying; Lam, Kin S.; Sorenson, Margaret E.; Wichtowski, John A.; Connolly, Timothy P.; Ueda, Yasutsugu; Bronson, Joanne J.; Zhang, Yunhui; Kim, Oak K.

PA Bristol-Myers Squibb Company, USA

SO PCT Int. Appl., 90 pp. CODEN: PIXXD2

DT Patent

T 75 English

	CNT 1										
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE						
PI	WO 2002014354	A1	20020221	WO 2001-US25560	20010815						
	W: AE, AG,	AL, AM,	AT, AU, AZ,	BA, BB, BG, BR, BY,	BZ, CA, CH, CN,						
	CO, CR,	CU, CZ,	DE, DK, DM,	DZ, EC, EE, ES, FI,	GB, GD, GE, GH,						
	GM, HR,	HU, ID,	IL, IN, IS,	JP, KE, KG, KP, KR,	KZ, LC, LK, LR,						
	LS, LT,	LU, LV,	MA, MD, MG,	MK, MN, MW, MX, MZ,	NO, NZ, PL, PT,						
	RO, RU,	SD, SE,	SG, SI, SK,	SL, TJ, TM, TR, TT,	TZ, UA, UG, UZ,						
	VN, YU,	ZA, ZW, .	AM, AZ, BY,	KG, KZ, MD, RU, TJ,	TM						
	RW: GH, GM,	KE, LS,	MW, MZ, SD,	SL, SZ, TZ, UG, ZW,	AT, BE, CH, CY,						
	DE, DK,	ES, FI,	FR, GB, GR,	IE, IT, LU, MC, NL,	PT, SE, TR, BF,						
	BJ, CF,	CG, CI,	CM, GA, GN,	GQ, GW, ML, MR, NE,	SN, TD, TG						
	US 2002065219	A1	20020530	US 2001-928468	20010813						
	AU 2001086497	A5	20020225	AU 2001-86497	20010815						
PRAI	US 2000-225598F	P	20000815								
	WO 2001-US25560	W	20010815								
OS	OS MARPAT 136:200481										

- AB Novel thiazolyl peptides R1-Y-CH2CH(O)CONHZ [Q is a residue of a thiazolyl peptide antibiotic, e.g., nocathiacin I or nosiheptide; Y = S, SO, SOC or NR, where R = H, OH, alkoxy, alkanoyl, alkylcarbamoyl, etc.; R1 = 1-azabicyclo[2.2.2]oct-3-yl or N-oxide, [(CH2)20]1-3(CH2)2R4' (R4' = OH, amino, phenylmethyl), or (un)substituted alkyl) were prepared for use in pharmaceutical compns. for the treatment of serious bacterial infections. Thus, a peptide prepared by Michael addition reaction of nocathiacin I with 1-methylpiperazine showed in vitro antibiotic activity 0.25, 0.125, and 0.5 µg/mL (MIC) against Staphylococcus aureus, Streptococcus pneumoniae, and Enterococcus faecalis, resp.
- IT 401826-04-8P 401826-37-7P 401826-74-2P
  RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
  (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
  (Uses)

(preparation of water-soluble thiazolyl peptide derivs.)

RN 401826-04-8 CAPLUS
04 - Thiazolecarboxamide, N-[2-amino-1-[[[2-(2,5-dioxo-1pyrrolidinyl) ethyl]amino]methyl]-2-oxoethyl]-2-[(118,14E,218,22R,33S,49S)9,10,11,21,31,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11[(1R)-1-hydroxyethyl]-14-(1-methoxyethylidien)-9,12,19,30,40,48-hexaoxo-49[(2,4,6-trideoxy-4-(dimethylamino)-3-C-methyl-a-1-lyxohexopyranosyl]oxy]-22,25-(ethanoxymethano)-8,5118,15:37,34-trinitrilo21,33-([2,4]-endo-thiazolomethanimino)-5H,15H,24H,34Hpyrido[37,21:20,21][1,28,8,18,24,4,11,14]dioxatritiatriazacyclodotriacont
ino[30,31-b]indol-2-yl]-(9C1) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 401826-37-7 CAPLUS

CN 4-Thiazolecarboxamide, N-[2-amino-1-[[methyl[2-(1-piperidinyl)ethyl]amino]methyl]-2-coxoethyl]-2-[(118,14E,218,22R,338,498)-9,10,11,12,13,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11-[(1R)-1-hydroxyethyl]-14-(1-methoxyethyl)dene)-9,12,19,30,40,48-hexaoxo-49-[[2,4,6-trideoxy-4-(dimethylamino)-3-C-methyl-α-1-lyxo-hexopyranosyl]oxy]-22,25-(ethanoxymethano)-8,5:18,15:37,34-trinitrilo-21,33-([2,4]-and-thiazolomethanimino)-5H,15H,24H,34H-pyrido[3',2':20,21][1,28,8,18,24,4,11,14]dioxatrithiatriazacyclodotriacontino[30,31-b]indol-2-yl]-(9CI) (CA INDEX NAME)

PAGE 2-A

PAGE 3-A

RN 401826-74-2 CAPLUS

CN 4-Thiazolecarboxamide, N-[2-amino-1-[[[3-(4-methyl-1-piperaziny])propy]amino]methyl]-2-coxoathyl]-2-[[118,148,218,228,338,498)-9,10,11,12,13,14,19,20,21,22,29,30,32,33-tetradecahydro-3,29-dihydroxy-11-[(18)-1-hydroxyethyl]-14-(1-methoxyethyl]dene)-9,12,19,30,40,48-hexaoxo-49-[[2,4,6-trideoxy-4-dimethylamino)-3-C-methyl-a-L-lyxo-hexopyranosyl]oxy]-22,25-(ethanoxymethano)-8,5:18,15:37,34-trinitrilo-21,33-([2,4]-endo-thiazolomethanimino)-5H,15H,24H,34H-pyrido[3',2':20,21][1,28,8,18,24,4,11,14]dioxatrithiatriazacyclodotriacontino[30,31-b]indol-2-yl]-(9(VI)) (CA INDEX NAME)

PAGE 1-A

PAGE 3-A

PAGE 4-A

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2000:643793 CAPLUS

DN 133:329128

TI Non-glutamate type pyrrolo[2,3-d]pyrimidine antifolates. III. Synthesis and biological properties of No-masked ornithine analogs

AU Itoh, Fumio; Yoshioka, Yoshio; Yukishige, Koichi; Yoshida, Sei; Ootsu, Koichiro; Akimoto, Hiroshi

CS Medicinal Chemistry Research Laboratories, Takeda Chemical Industries, Ltd., Osaka, 532-8686, Japan

SO Chemical & Pharmaceutical Bulletin (2000), 48(9), 1270-1280

CODEN: CPBTAL; ISSN: 0009-2363
PB Pharmaceutical Society of Japan

DT Journal

LA English

CASREACT 133:329128

OS GI

$$\begin{array}{c|c} & \text{NH2} & \text{CCH2})_m & \text{CO2H} \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & \\ & & \\ & \\ & \\ & & \\ & \\ & & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ & \\ &$$

AB Non-glutamate type pyrrolo[2,3-d]pyrimidine antifolates I [m = 2,3; n = 1-4; R = H, CO2Bu-t, CO2CH2Ph, CO(CH2)2CO2H, COCH:CHCO2H, COCGH4CO2H-2, COCGH4CO2H-3, C-(1-pyrrolidinylcarbonyl)benzoyl, COCGH4OH-2, COCGH4(NHAc)-4, SO2CGH4CO2H-3, SO2CGH4CO2H-2, CONHCGH4F-4, CONHCGH4-3B(DA)3, CGH4CO2H-3, SO2CGH4CO2H-2, CONHCGH4F-4, CONHCGH4-3B(DA)3, CGH4CO2H-3, SO2CGH4CO2H-2, CONHCGH4F-4, CONHCGH4-3B(DA)4, CGH4CO2H-3, SO2CGH4CO2H-2, CONHCGH4F-4, CONHCGH4CO2H-3, CONHCGH4-3B(DA)4, CHC and their inhibitory effects on dihydrofolate reductase (DHFR), the growth of murine fibrosarcoma Meth A cells, and methotrexate-resistant human CCRF-CEM cells were examined A free ornithine analog I (m = n = 3, R = H) did not strongly inhibit Meth A cell growth, whereas all No-substituted ornithine analogs (R = acyl, sulfonyl, carbamoyl, aryl) exhibited much more potent inhibitory activities against both DHFR and Meth A cell growth. In particular, compds. I [m = 2, n = 3,

Ι

 $R = COG6H4CO2H-2; \ m = 2, \ n = 3, \ R = 3-carboxy-2-naphthoyl; \ m = 2, \ n = 3, \ R = C6H4CO2H-3] \ also showed remarkable growth-inhibitory activities against methotrexate-resistant CCRF-CEM cells. These results demonstrate that the potent inhibitory activities of No-masked ornithine analogs against the growth of Meth A cells and methotrexate-resistant CCRF-CEM cells, results from effective uptake via reduced folate carrier and their potent DHFR inhibition.$ 

T 149009-83-6P 303957-87-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and antitumor activity of non-glutamate, ornithine-containing pyrrolo[2,3-d]pyrimidine antifolates)

RN 149009-83-6 CAPLUS

2H-Isoindole-2-hexanoic acid,  $\alpha$ -[[4-[3-(2,4-diamino-1H-pyrrolo[2,3-d]pyrimidin-5-yl)propyl]benzoyl]amino]-1,3-dihydro-1,3-dioxo-, methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 303957-87-1 CAPLUS

CN 2H-Isoindole-2-hexanoic acid, a-[[4-[2-(2,4-diamino-1H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]amino]-1,3-dihydro-1,3-dioxo-, methyl ester, (aS)-(9CI) (CA INDEX NAME)

PAGE 1-B

THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 29 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L6
    ANSWER 12 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
```

AN 2000:260225 CAPLUS

DN 132:294010

ΤI Preparation of diaminopropionic acid derivatives as intracellular adhesion molecule-1 (ICAM-1) binding inhibitors

IN Fotouhi, Nader; Gillespie, Paul; Guthrie, Robert William; Pietranico-Cole, Sherrie Lynn; Yun, Weiya

F. Hoffmann-La Roche A.-G., Switz. PA

SO PCT Int. Appl., 259 pp.

CODEN: PIXXD2

DT Patent.

LA	Engli	sh.															
FAN.	CNT 1																
	PATEN	r NO.			KIN	D	DATE			APPL	ICAT	ION I	NO.		D.	ATE	
PI	WO 20	000219	20		A1		2000	0420		WO 1	999-	EP76:	20		1	9991	012
	W	AE,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,
		DE,	DK,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,
		JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,
		MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,
		ТJ,	TM,	TR,	TT,	UA,	UG,	UZ,	VN,	YU,	ZA,	ZW					
	R	√: GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,
		DK,	ES,	FΙ,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,
		CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG				
	US 63	31640			B1		2001	1218		US 1	999-	4075	34		1	9990	929
	CA 23	14058			A1		2000	0420		CA 1	999-	2344	058		1	9991	012

	BR	9914	602			A		2001	0703		BR	19	99-	1460	2		1	9991	012
	EP	1121	342			A1		2001	8080		EP	19	99-	9537	72		13	9991	012
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GF	۲,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
			IE,	SI,	LT,	LV,	FI,	RO											
	TR	2001	0103	8		T2		2001	0921		TR	20	01-	1038			1	9991	012
	JΡ	2002	5274	16		T		2002	0827		JP	20	00-	5758	29		1	9991	012
	JP	3720	709			B2		2005	1130										
	AU	7664	68			В2		2003	1016		ΑU	20	00-	1034	9		1	9991	012
	MX	2001	PA03	284		A		2001	1011		MX	20	01-	PA32	84		2	010	329
	ZA	2001	0026	08		A		2002	0930		za	20	01-	2608			2	0010	329
	US	2002	0525	12		A1		2002	0502		US	20	01-	8797	00		2	010	612
	US	2004	0062	36		A1		2004	0108		US	20	03-	3492	89		2	0030	122
	US	6803	384			B2		2004	1012										
	US	2005	0801	19		A1		2005	0414		US	20	04-	9456	50		2	0040	921
	US	7217	728			B2		2007	0515										
	US	2007	1556	71		A1		2007	0705		US	20	07-	7039	25		2	0070	208
PRAI		1998				P		1998											
		1999				A3		1999	0929										
	WO	1999	-EP7	620		W		1999	1012										
		2001				В3		2001											
	US	2003	-349	289		A3		2003	122										
	US	2004	-945	650		A3		2004	921										
OS	MAI	RPAT	132:	2940	10														
CT																			

$$\begin{array}{c} \text{CONHCH} & \text{CH}_2-\text{NH}-\text{X-}(Y)_{m}-\text{Z} \\ \text{CO}_2\text{H} & \text{V} \end{array}$$

AB Diaminopropionic acid derivs. I [R1 = substituted 1-naphthyl, 4-indolyl, 4-benzimidazolyl, 4-benzodiazolyl, 4-benzotriazolyl, or phenyl; R2 = CHR3NHCO (R3 = H, carboxy, alkyl), CH2CH2CO, 1,2-cyclopropanediylcarbonyl, OCH2CO, CH:CHCHR3, CH2CH2CH(OH), CONHCHR3, or CH2NH-5,1-tetrazolediy1; U, V, W = H, halo, alkyl provided that U and V are not both hydrogen; X = CO, phenylalkylene, sulfonyl; Y = alkylene which may be substituted by amino or cycloalkyl, alkenylene, alkylenethio; Z = H, alkylthio, CO2H, CONH2, 1-adamantyl, diphenylmethyl, 3-[[(5-chloro-2-pyridinyl)amino]carbonyl]-2pyrazinyl, hydroxy, phenylmethoxy, 2-chloro-4-[[[(3hvdroxvphenvl)methyl]amino]carbonyl]phenyl, [(2,6-dichlorophenyl)methoxy], Ph, (un) substituted cycloalkyl or aryl or fused ring system which may contain 0-3 heteroatoms; m, n = 0, 1] or their pharmaceutically acceptable salts or esters were prepared and are useful for treating rheumatoid arthritis, psoriasis, multiple sclerosis, Crohn's disease, ulcerative colitis, atherosclerosis, restenosis, pancreatitis, transplant rejection, delayed graft function and diseases of ischemia reperfusion injury, including acute myocardial infarction and stroke. Thus, N-[2-chloro-4-[[[(3-hydroxyphenyl)methyl]amino]carbonyl]benzoyl]-3-(3methoxybenzoylamino)-L-alanine was prepared by the solid-phase method and showed IC50 = 1.2 nM in the LFA-1 (lymphocyte function-associated

Ι

antigen-1)/ICAM-1 protein-protein assav.

IT 264273-57-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diaminopropionic acid derivs. as intracellular adhesion mol.-1 (ICAM-1) binding inhibitors)

RN 264273-57-6 CAPLUS

CN L-Alanine, N-[2-chloro-4-[[[(3-hydroxyphenyl)methyl]amino]carbonyl]benzoyl ]-3-[[1-oxo-3-(1-piperidinyl)propyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L6 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN AN 2000:175829 CAPLUS DN 132:208143 TI Preparation of peptides as NK-1 receptor antagonists
```

IN Groger, Karsten; Sisto, Alessandro

PA Menarini Ricerche S.p.A., Italy

SO PCT Int. Appl., 43 pp. CODEN: PIXXD2

DT Patent LA English

FAN.		1																
	PA:	TENT :	NO.			KIN	D	DATE			APPL	ICAT	I NOI	NO.		D.	ATE	
							-									-		
PI	WO	2000	0141	09		A1		2000	0316		WO 1	999-1	EP65	41		1	99909	906
		W:	ΑE,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
			CZ,	DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	HU,	ID,	IL,
			IN,	IS,	JP,	KE,	KG,	KP,	KR,	KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,
			MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,
			SL,	ΤJ,	TM,	TR,	TT,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,
			KG,	KZ,	MD,	RU,	ТJ,	TM										
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SL,	SZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	DK,
			ES,	FΙ,	FR,	GB,	GR,	IE,	ΙT,	LU,	MC,	NL,	PT,	SE,	BF,	ΒJ,	CF,	CG,
			CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG					
	IT	1304	898			B1		2001	0405		IT 1	998-1	FI20	1		1	99809	908
	AU	9957	457			A1		2000	0327		AU 1	999-	5745	7		1	99909	906
PRAI		1998						1998	0908									
	WO	1999	-EP6	541		W		1999	0906									

OS MARPAT 132:208143

AB Peptides R1(CH2)nCONHCH[(CH2)pR2]CONHCHR3CONR4R5 [(S)-configuration at

CHR3, n = 0-3; p = 0-4; R1 = a basic moiety chosen from an amino or heterocyclyl group, aryl or arylalkyl which can be substituted on the aromatic moiety; R2 = R6(CH2)m-X1-, where m = 0-3; R6 = amino group, heterocyclyl, aryl or arylalkyl which can be substituted on the aromatic moiety; X1 = CONH or NHCO; R3 = naphthylmethyl, halobenzyl, indolylmethyl; R4 = aryl or arylalkyl which can be substituted on the aromatic moiety; R5 = H, M6] (with provisos) were prepared as NR-1 receptor antagonists. Thus, Na-(Na-(1H)indol-3-ylcarbonyl)-L-asparaginyl[B-N-[2-(morpholin-4-yl)ethyl])-L-[3,4-dichlorophenyl)alanine]-N-methyl-N-(4-bromobenzyl)amide, prepared by step-wise couplings in solution, showed pKi = 9.3 for inhibition of [3H]SP binding to 1M9 cells.

IT 260809-08-3P 260809-12-9P 260809-13-0P 260809-14-1P 260809-16-3P 260809-17-4P 260809-18-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of peptides as NK-1 receptor antagonists)

RN 260809-08-3 CAPLUS

CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[1-oxo-3-(1-piperidinyl)propyl]amino]-L-alanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

RN 260809-12-9 CAPLUS

CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[3-(4-methyl-1-piperazinyl)-1-oxopropyl]amino]-L-alanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

- RN 260809-13-0 CAPLUS
- CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[1-oxo-3-(1-piperidinyl)propyl]amino]-L-alanyl-N-methyl-3-(2-naphthalenyl)-N-(phenylmethyl)- (9C1) (CA INDEX NAME)

Absolute stereochemistry.

- RN 260809-14-1 CAPLUS
- CN L-Tryptophanamide, N-(1H-indol-3-ylcarbonyl)-3-[[1-oxo-3-(1piperidinyl)propyl]amino]-L-alanyl-N-methyl-N-[(4-methylphenyl)methyl](SCI) (CA INDEX NAME)

- RN 260809-16-3 CAPLUS
- CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[1-oxo-3-(1piperidinyl)propyl)aminol-D-alanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

## Absolute stereochemistry.

- RN 260809-17-4 CAPLUS
- CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[[3-(4-methyl-1-piperazinyl)-1-oxpropyl]amino]-D-alanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9C1) (CA INDEX NAME)

RN 260809-18-5 CAPLUS

CN L-Alaninamide, N-(1H-indol-3-ylcarbonyl)-3-[(1-piperazinylacetyl)amino]-Dalanyl-N-methyl-N-[(4-methylphenyl)methyl]-3-(2-naphthalenyl)- (9CI) (CA
INDEX NAME)

# Absolute stereochemistry.

# RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L6 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 1997:53583 CAPLUS
- DN 126:70149
- TI Hydrochlorides of 1-phenyl-1-(p-nitrobenzoyl amino)-5-(n-piperidino)- or (n-diethylamino)pentanes having antiarrhythmic and antifibrillation activity
- IN Mashkovskij, M. D.; Glushkov, R. G.; Skachilova, S. Ya.; Dorodnikova, E. V.; Rozenshtraukh, L. V.; Voronin, V. G.; Zheltukhin, N. K.; Anyukhovskij, E. P.; Nesterenko, V. V.; Cherkasova, E. M.

## 10/539372

- PΆ Tsentr Po Khimii Lekarstvennykh Sredstv, USSR; Vsesoyuznyj Nauchnyj Tsentr Po Bezopasnosti Biologicheski Aktivnykh Veshchesty: Vsesovuznyi Kardiologicheskij Nauchnyj Tsentr Amn Sssr
- U.S.S.R. From: Izobreteniya 1996, (6), 261. CODEN: URXXAF

Patent

T.A Russian

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	SU 1833612 SU 1987-4359472	A3	19960227 19871208	SU 1987-4359472	19871208		
	Title only translat	ed.	17071200				

ΙT 185384-75-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(Hydrochlorides of 1-phenyl-1-(p-nitrobenzovl amino)-5-(n-piperidino)or (n-diethylamino)pentanes having antiarrhythmic and antifibrillation activity)

RN 185384-75-2 CAPLUS

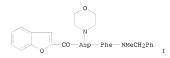
CN Benzamide, 4-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]-, monohydrochloride (9CI) (CA INDEX NAME)

# ■ HC1

- L6 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 1996:494173 CAPLUS
- DN 125:143330
- TΙ Peptide compounds for prevention and/or treatment of nitric oxide
- (NO)-mediated diseases
- Itoh, Yoshikuni; Iwamoto, Toshiro; Yatabe, Takumi; Hamashima, Hitoshi; TN Inoue, Takayuki; Hashimoto, Seiji; Oku, Teruo
- Fujisawa Pharmaceutical Co., Ltd., Japan PA
- PCT Int. Appl., 739 pp. SO
- CODEN: PIXXD2
- DT Patent
- LA English
- FAN. CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9616981	A2	19960606	WO 1995-JP2428	19951129
	WO 9616981	A3	19960906		
	W: AH, CA, CN,	FT. HO	. JP. KR. MX	C. NO. NZ. RU. UA. US	

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG AU 1995-39937 AU 9539937 Α 19960619 19951129 EP 796270 A2 19970924 EP 1995-938602 19951129 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE ZA 9510201 A 19960625 ZA 1995-10201 19951130 US 1997-849076 US 5932737 Α 19990803 19970530 PRAI GB 1994-24408 Α 19941202 GB 1995-4891 Α 19950310 GB 1995-10042 Α 19950518 WO 1995-JP2428 19951129 OS MARPAT 125:143330



- AB Peptides WAINRSCH(A2T)CONR9CH(A3R3)R4 [W = alkyl, (un)substituted aryl or fluorenyl, etc.; Al = alkylene, NHCO, CO, CS, SO2; A2 = alkylene; T = H, aryl, heterocyclyl, OH, etc.; R8 = H, alkyl; R8 may link with A2T to form CH2C6H4CH2-O (Q); A3 = bond, alkylene; R3 = H, aryl, OH, etc.; R9 = H, alkyl or may link with A3R3 to form Q; R4 = CO2H, protected carboxy, carboxamido, etc. or CH(A3R3)R4 = N-alkyl-2-oxoquinoline moiety) or their pharmaceutically acceptable salts were prepared for use as medicaments. Thus, dipeptide I was prepared by acylation of aspartylphenylalaninamide derivative with 2-benzofurancarboxylic acid. I and six other peptides showed 100% inhibition of NO production in tests of murine macrophage cells.
- RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of peptides for prevention and/or treatment of nitric oxide-mediated diseases)
- RN 179881-40-4 CAPLUS
  CN L-Phenylalaninamide, N-(2-benzofuranylcarbonyl)-O-(4-pyridinylacetyl)-Lseryl-N-methyl-N-(phenylmethyl)- (9C1) (CA INDEX NAME)

179881-43-7 CAPLUS

CN L-Phenylalaninamide, N-(2-benzofuranylcarbonyl)-0-[1-oxo-3-(1piperidinvl)propvl]-L-servl-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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ANSWER 16 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
L6
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1995:904875 CAPLUS AN

DN 124:240

TΙ Search for antiarrhythmic drugs among 1,5-diaminopentane derivatives

ΑIJ Mashkovskii, M. D.; Glushkov, R. G.; Dorodnikova, E. V.; Yuzhakov, S. D.

CS TSKhLS, VNIKhFI, Moscow, Russia

SO Khimiko-Farmatsevticheskii Zhurnal (1995), 29(3), 27-31 CODEN: KHFZAN; ISSN: 0023-1134

PB Meditsina

DT Journal

LA Russian

AB Most of the 28 1,5-diaminopentanes tested showed antiarrhythmic activity in rats. Structure-activity relations are briefly discussed.  $171203-85-3\ 171203-86-4\ 171203-87-5$ 

171203-88-6 171203-89-7 171203-90-0

171203-91-1 171203-92-2 171203-93-3

171203-94-4 171203-95-5 171203-96-6

171203-99-9 171204-00-5 171204-01-6

171204-02-7 171204-03-8 171204-04-9

171204-05-0 171204-06-1 171204-07-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(search for antiarrythmic drugs among 1,5-diaminopentane derivs.)

RN 171203-85-3 CAPLUS

CN Benzamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{O} \\ & | & | & | \\ & \text{CH}_2) \, _4-\text{CH}-\text{NH}-\text{C}-\text{Ph} \end{array}$$

RN 171203-86-4 CAPLUS

CN 3-Pyridinecarboxylic acid, compd. with N-[1-phenyl-5-(1-piperidinyl)pentyl]benzamide (1:1) (9CI) (CA INDEX NAME)

CM :

CRN 171203-85-3 CMF C23 H30 N2 O

$$\begin{array}{c|c} & \text{Ph} & \text{O} \\ & | & | \\ \text{CH}_2)_4 - \text{CH} - \text{NH} - \text{C} - \text{Ph} \end{array}$$

CM 2

CRN 59-67-6 CMF C6 H5 N O2

RN 171203-87-5 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-2,6-dioxo-, compd. with N-[1-phenyl-5-(1-piperidinyl)pentyl]benzamide (1:1) (CA INDEX NAME)

CM 1

CRN 171203-85-3 CMF C23 H30 N2 O

$$\begin{array}{c|c} & \text{Ph} & \text{O} \\ & | & | \\ \text{CH-NH-C-Ph} \end{array}$$

CM 2

CRN 65-86-1 CMF C5 H4 N2 O4

RN 171203-88-6 CAPLUS

CN Benzamide, N-[1-(4-methylphenyl)-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

RN 171203-89-7 CAPLUS

CN Benzamide, N-[1-(4-chlorophenyl)-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

RN 171203-90-0 CAPLUS

CN Benzamide, 4-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

RN 171203-91-1 CAPLUS

CN Benzamide, N-[1-(4-methylphenyl)-5-(1-piperidinyl)pentyl]-4-nitro- (CA INDEX NAME)

RN 171203-92-2 CAPLUS

CN Benzamide, N-methyl-4-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

RN 171203-93-3 CAPLUS

CN Benzamide, N-[1-[4-(1-methylethyl)phenyl]-5-(1-piperidinyl)pentyl]-4-nitro-(CA INDEX NAME)

RN 171203-94-4 CAPLUS

CN Benzamide, N-[1-(4-methoxyphenyl)-5-(1-piperidinyl)pentyl]-4-nitro- (CA INDEX NAME)

RN 171203-95-5 CAPLUS

CN Benzamide, N-[1-(3,4-dimethylphenyl)-5-(1-piperidinyl)pentyl]-4-nitro-(CA INDEX NAME)

RN 171203-96-6 CAPLUS

CN Benzamide, N-[1-(3,4-dimethoxyphenyl)-5-(1-piperidinyl)pentyl]-4-nitro-(CA INDEX NAME)

RN 171203-99-9 CAPLUS

CN Benzamide, N-[5-(4-methyl-1-piperazinyl)-1-phenylpentyl]-4-nitro-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

- RN 171204-00-5 CAPLUS
- CN Benzamide, 4-bromo-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

- RN 171204-01-6 CAPLUS
- CN Benzamide, 2,4-dinitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

- RN 171204-02-7 CAPLUS
- CN Benzamide, 2-chloro-5-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

- RN 171204-03-8 CAPLUS
- CN Benzamide, 2,4-dichloro-N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

RN 171204-04-9 CAPLUS

CN Benzamide, 3,4,5-trimethoxy-N-[1-pheny1-5-(1-piperidiny1)penty1]- (CA INDEX NAME)

RN 171204-05-0 CAPLUS

CN 4-Pyridinecarboxamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{O} \\ & \text{N} & \text{(CH}_2)_4 - \text{CH} - \text{NH} - \text{C} \end{array}$$

# ●2 HC1

RN 171204-06-1 CAPLUS

CN 3-Pyridinecarboxamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]- (CA INDEX NAME)

RN 171204-07-2 CAPLUS

- L6 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 1994:605936 CAPLUS
- DN 121:205936
- TI Synthesis and Biological Activity of No-Hemiphthaloyla, o-diaminoalkanoic Acid Analogs of Aminopterin and 3',5-Dichloroaminopterin
- AU Rosowsky, Andre; Bader, Henry; Wright, Joel E.; Keyomarsi, Khandan; Matherly, Larry H.
- CS Dana-Farber Cancer Institute, Harvard Medical School, Boston, MA, 02115,
- SO Journal of Medicinal Chemistry (1994), 37(14), 2167-74 CODEN: JMCMAR; ISSN: 0022-2623
- DT Journal
- LA English
- GI

AB Analogs of Nα-(4-amino-4-deoxypteroyl)-Nδ-(hemiphthaloyl)-Lornithine (I) (ET523) with 3',5'-dichloro substitution in the p-aminobenzoyl moiety or with one less or more CH2 group in the amino acid moiety were synthesized and tested as inhibitors of dihydrofolate reductase (DHFR) activity and cell growth. Replacement of L-ornithine in I by L-2,4-diaminobutanoic acid or L-lysine did not decrease binding to human recombinant DHFR but resulted in some loss of activity against SCC25 human and SCC VII murine squamous cell carcinoma and against MCF-7 human breast carcinoma in culture. PT523 was several times more potent than methotrexate (MTX), aminopterin (AMT), or trimetrexate (TMQ). 3',5'-Dichloro substitution did not decrease either DHFR binding or cytotoxicity. A new synthetic route to I from 2,4-diamino-6-(hydroxymethyl)pteridine and Nα-(4-aminobenzoyl)-Nδ-phthaloyl-L-ornithinine Me ester was investigated but was not superior to previously described methods. In comparative expts. on the ability of PT523 and MTX to competitively inhibit the influx of (6R)-5,10-dideazatetrahydrofolate (DDATHF, lometrexol), used a surrogate for MTX and reduced folates, the Ki of PT523 was lower than that of MTX in both wild-type CCRF-CEM human leukemic lymphoblasts and the transport- and polyglutamylation-defective subline CEM/MTX. The CCRF-CEM cells were 10-fold more sensitive to PT523 than to MTX, whereas the CEM/MTX cells were 240-fold more sensitive. However, in contrast to other MTX-resistant cells where collateral sensitivity to PT523 has been seen. CEM/MTX cells still showed substantial cross resistance to PT523 which may reflect an unusual heightened ability to utilize exogenous folic acid. The good correlation observed with both cell lines between the cytotoxicity of PT523 and MTX and the ability to inhibit DDATHF influx supported the view that PT523 and MTX share, at least in part, a common protein carrier for membrane transport. 158090-66-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, saponification, and imide ring opening of)

158090-66-5 CAPLUS RN

CN 2H-Isoindole-2-hexanoic acid, α-[[4-[[(2,4-diamino-6pteridinyl)methyl|formylamino|benzoyl|amino|-1,3-dihydro-1,3-dioxo-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

```
1.6
     ANSWER 18 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
```

1993:626417 CAPLUS AN

119:226417 DN

TΙ Preparation of condensed pyrimidinylacyl amino acids as neoplasm inhibitors ΙN

Akimoto, Hiroshi; Ootsu, Koichiro; Itoh, Fumio PA Takeda Chemical Industries, Ltd., Japan

SO Eur. Pat. Appl., 51 pp.

CODEN: EPXXDW

DT Pat.ent.

LA

English

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI	EP 530537	A1 19930310	EP 1992-113523	19920807
	EP 530537	B1 19970108		
	R: AT, BE, CH,	DE, DK, ES, FR, G	B, GR, IE, IT, LI, LU,	NL, PT, SE
	US 5403843	A 19950404	US 1992-926170	19920807
	AT 147386	T 19970115	AT 1992-113523	19920807
	CA 2075787	A1 19930213	CA 1992-2075787	19920811
	JP 06049069	A 19940222	JP 1992-214142	19920811
	JP 3376479	B2 20030210		
PRAI	JP 1991-202042	A 19910812		
	JP 1992-71513	A 19920327		
	JP 1992-145851	A 19920605		
OS	CASREACT 119:226417		.7	
GI	For diagram(s), see	printed CA Issue.		
AB			ed) (hydrogenated) 5-me	embered ring:
			ered homo- or heterocyc	
			on C bandad anaus.	

Title compds. [I; ring A = (substituted) (hydrogenated) 5-membered ring; B = (substituted) divalent 5- or 6-membered homo- or heterocyclic group; X = amino, OH, SH; Y = H, halo, C-, N-, O-, or S-bonded group; Z = (substituted) (heteroatom-containing) divalent group having ≤5 atoms; W = NRCO; R = H, (substituted) alkyl; R1 = (substituted) cyclic or chain-like group; or RR1 = atoms to form a 3-13 membered ring COZR2 = optionally esterified carboxyl group; p = 1-4; with provisos], were prepared Thus, Nw-[4-[2-(2,4-diamino-7H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]-Nδ-phthaloyl-L-ornithine Me ester [prepared by condensation of the corresponding benzoic acid with Nδ-phthaloyl-L-ornithine Me ester.HCl using di-Et cyanophosphate and Et3N in DMT] was saponified to give Nw-[4-[2-(2,4-diamino-7H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoyl]-Nδ-hemiphthaloyl-L-ornithine. This inhibited proliferation of A549 cells with LCSO = 0.0012 us/nL.

IT 149009-83-6P

RI: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREF (Preparation)

(preparation of, as neoplasm inhibitor)

RN 149009-83-6 CAPLUS

CN 2H-Isoindole-2-hexanoic acid, α-[[4-[3-(2,4-diamino-1H-pyrrolo[2,3-d]pyrimidin-5-yl)propyl]benzoyl]amino]-1,3-dihydro-1,3-dioxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

L6 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1993:603167 CAPLUS

DN 119:203167

TI Substituted 1-phenyl-1-benzoylamino-5-aminopentanes, their preparation and use

IN Mashkovsky, Mikhail D.; Glushkov, Robert G.; Skachilova, Sofiya Y.; Dorodnikova, Elena V.; Rosenshtraukh, Leonid V.; Voronin, Vasily G.; Zheltukhin, Nikolai K.; Anjukhovsky, Evgenii P.; Nesterenko, Vladislav V.; et al.

PA USSR

SO Can. Pat. Appl., 12 pp.

CODEN: CPXXEB

DT Patent LA English

FAN.CNT 1

		PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
	PI	CA 2073833	A1	19930301	CA 1992-2073833	19920714	
		EP 535256	A1	19930407	EP 1991-114635	19910830	
		R: AT, BE, CH,	DE, DK	, ES, FR, GB	, IT, LI, NL, SE		
		HU 62854	A2	19930628	HU 1992-2316	19920714	
		ZA 9205237	A	19940114	ZA 1992-5237	19920714	
		AU 9220407	A	19930304	AU 1992-20407	19920720	
		AU 648422	B2	19940421			
		BR 9202849	A	19930406	BR 1992-2849	19920723	
		JP 06192197	A	19940712	JP 1992-226829	19920826	
	PRAI	EP 1991-114635	A	19910830			
	os	CASREACT 119:203167	; MARPA	T 119:203167			
	CT						

AB The title compds. (I; R1 = halo, N02, C1-4 aminoacyl, sulfonamido; R2, R3 = C1-5 alkyl or R2R3 = C3-6 alkylene) and their optically active isomers and their physiol. tolerated acids are prepared as antiarrhythmic and

antifibrillatory compds. [e.g., (t)-I (R1 = p-NO2, R2 = R3 = Et). HC1 ((±)-II); (+)- and (-)-II). Thus, Et2N(CH2)4CH(NH2)Ph.HCl in 10% aqueous NaOH-Me2CO is treated with p-02NC6H4COC1 to give I (R1 = p-N02, R2 = R3 = Et); this in Me2CO with HCl in Me2CHOH gives (±)-II. Dosages are given.

- IT 150492-00-5 150492-01-6 185384-75-2 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation as antiarrythmic)
- RN 150492-00-5 CAPLUS
- CN Benzamide, 4-bromo-N-[1-phenyl-5-(1-piperidinyl)pentyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

- RN 150492-01-6 CAPLUS
- CN Benzamide, 4-(acetylamino)-N-[1-phenyl-5-(1-piperidinyl)pentyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

- RN 185384-75-2 CAPLUS
- CN Benzamide, 4-nitro-N-[1-phenyl-5-(1-piperidinyl)pentyl]-, monohydrochloride (9CI) (CA INDEX NAME)

## ● HCl

ANSWER 20 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1991:229364 CAPLUS

DN 114:229364

ΤI Synthesis of  $\alpha$ ,  $\omega$ -diamino acids via amidocarbonylation reaction: novel synthesis of lysine, ornithine, and their analogs.

Amino, Yusuke; Izawa, Kunisuke

CS Cent. Res. Lab., Ajinomoto Co., Inc., Kawasaki, 210, Japan SO Bulletin of the Chemical Society of Japan (1991), 64(2), 613-19 CODEN: BCSJA8; ISSN: 0009-2673

Journal

LA English

os CASREACT 114:229364

 $\alpha, \omega$ -Diamino acid derivs., and as lysine and ornithine, were synthesized via cobalt-catalyzed amidocarbonylation of m-(phthalimido)alkanals in good yield. The phthalimido group was stable to the conditions of amidocarbonylation. The hydroformylationamidocarbonylation of N-phthalov1-B, y- and N-phthalov1γ, δ-unsatd. amines proceeds very nicely to give α, ω-diamino acids with good selectivity. Selective deprotection of α-N-acyl-ω-N-phthaloyl α,ω-amino acids was achieved using hydrazine for the N-phthaloyl group and aminoacylase for the N-acetyl group to afford the optically active α, ω-diamino acid. ΙT

133787-09-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 133787-09-4 CAPLUS

2H-Isoindole-2-hexanoic acid,  $\alpha$ -(benzoylamino)-1,3-dihydro-1,3-dioxo-CN , methyl ester (CA INDEX NAME)

## 10/539372

- ANSWER 21 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN 1.6 1973;72548 CAPLUS
- AN
- 78:72548 DN

OREF 78:11545a,11548a

- N-Phthaloylation of chloro- and hydroxy-2-amino acids TI
- ΑU Clarke, S.; Hider, R. C.; John, D. I.
- CS Dep. Biochem., Yale Univ., New Haven, CT, USA
- SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), (3), 230-4 CODEN: JCPRB4; ISSN: 0300-922X
- DT Journal
- LA English
- OS. CASREACT 78:72548
- AR N-Phthaloylation of 4-chloro- and 4-hydroxy-2-amino acids was achieved in 40-88% yield with N-(ethoxycarbonyl)phthalimide (I) (1.1 equivalent) in Me2SO containing Et3N; thus prepared were the N-phthaloyl derivs. of C1(CH2)2-CH(NH2)CO2Me) (II), the Me esters of 3-chloroalanine, and 4-chloronorvaline, and the lactone of 4-hydroxyleucine. Phthaloylation of 4-chlorolysine Me ester gave 26% of the N6-phthaloyl and N, N'-diphthaloyl derivs. Similarly, phthaloylation of the lactone of 4-hydroxylysine gave a mixture of the N6-phthalovl and N.N'-diphthalovl derivs. The rates of cyclization of the intermediates o-(EtO2CNHCO)C6H4CONHR (R = C1(CH2)2-CHCO2Me, PhCH2, Bu) isolated from the reactions of I with II, PhCH2NH2, and BuNH2, resp., confirmed the mechanism proposed for aminolysis of I.
  - 39739-20-3P
  - RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
- RN 39739-20-3 CAPLUS
- CN 2H-Isoindole-2-hexanoic acid, α-(benzoylamino)-γ-chloro-1,3
  - dihydro-1,3-dioxo-, methyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

- ANSWER 22 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN L6
- AN 1963:33274 CAPLUS
- DN 58:33274
- OREF 58:5631d-a
- 1,5,9-Triaminononane derivatives
- AU Ose, Shinsuke; Takamatsu, Hideji; Saeki, Takeji
- Dai-nippon Pharm. Co., Osaka
- SO Yakugaku Zasshi (1962), 82, 1197-9 CODEN: YKKZAJ; ISSN: 0031-6903
- Journal

AR

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LA Unavailable
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g. BzCl 16 hrs. to give 20.1 g. 1,9-dibromo-5-benzamidononane (I), m.
    82-3° (ligroine). A solution of I in C6H6 is refluxed with Me2NH 15
    hrs. to give 1,9-bis(diethylamino)-5-benzamidononane (II), m.
    82-3°. Similarly prepared are the following [R(CH2)4]2CHNHBz (R and
    m.p. given): piperidino, 90-2°; morpholino, 98-101°;
    pyrroliding, 89-91°; 1,2,3,4-tetrahydro-2-isoguinolyl,
    111-12°; 1,2,3,4-tetrahydro-1-quinoly1, 134-5°. II is
    heated with 20 times excess H3PO4 at 180-5° 12 hrs. to give
    1,9-bis(diethylamino)-5-aminonane (III), sirupy. Similarly are prepared the
    following [R(CH2)4]2CHNH2R (R and b.p./mm. given): piperidino,
    186-7°/2; morpholino, 200-4°/3.5; pyrrolidino,
    162-3°/1; 1,2,3,4-tetrahydro-2-isoquinolyl, sirupy;
    1,2,3,4-tetrahydro-1-quinolyl, sirupy. III is heated with HCHO and HCO2H,
    made alkaline with NaOH, and extracted with Et20 to give
1,9-bis(diethylamino)-5-
    dimethylaminononane (IV), bl 118°; trihydrochloride m. 247°.
    Similarly are prepared the following [R(CH2)4]2CHNMe2 (R, b.p./mm., and m.p.
    of trihydrochloride given); piperidino, 177°/1, 256°;
    morpholino, 185°/2, 254-6°; pyrrolidino, 158-160°/1,
    230-1°: 1,2,3,4-tetrahydro-2-isoguinoly1, 250°/0,4,
    115-18°. IV is allowed to stand with MeBr in EtOH to give the
    corresponding methobromide, m. 267-8°(EtOH). Similarly prepared are
    following [R2MeN+(CH2)4]2CHN+ Me3.3Br- (R2N and m.p. given): piperidino,
    280-1°; morpholino, 259-60°; pyrrolidino, 277-8°;
    1,2,3,4-tetrahydro-2-isoguinolyl, 232-3°; 1,2,3,4-tetrahydro-1-
```

A solution of 21 g. 1,9-dibromo-5-aminononane-HCl in C6H6 is refluxed with 12

quinoly1, 133-6°. IT 96173-74-9P, Benzamide, N-[5-piperidino-1-(4-piperidinobuty1)penty1]- 96586-63-9P, Benzamide,

N-[5-(1-pyrrolidiny1)-1-[4-(1-pyrrolidiny1)buty1]penty1]-

97573-27-8P, Benzamide, N-[5-(3,4-dihydro-2(1H)-isoquinoly1)-1-[4-(3,4-dihydro-2(1H)-isoquinoly1)buty1]penty1]- 97573-28-9P,

Benzamide, N-[5-(3,4-dihydro-1(2H)-quinolyl)-1-[4-(3-4-dihydro-1(2H)-quinolyl)butyl]pentyl]-

RL: PREP (Preparation)
(preparation of)

- RN 96173-74-9 CAPLUS
- CN Benzamide, N-[5-piperidino-1-(4-piperidinobutyl)pentyl]- (7CI) (CA INDEX NAME)

- RN 96586-63-9 CAPLUS
- CN Benzamide, N-[5-(1-pyrrolidinyl)-1-[4-(1-pyrrolidinyl)butyl]pentyl]- (CA INDEX NAME)

RN 97573-27-8 CAPLUS

CN Benzamide, N-[5-(3,4-dihydro-2(1H)-isoquinoly1)-1-[4-(3,4-dihydro-2(1H)-isoquinoly1)buty1]penty1]- (7CI) (CA INDEX NAME)

RN 97573-28-9 CAPLUS

CN Benzamide, N-[5-(3,4-dihydro-1(2H)-quinoly1)-1-[4-(3,4-dihydro-1(2H)-quinoly1)buty1]penty1]- (7CI) (CA INDEX NAME)

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=> s 15 L7 1 L5

=> d 17 bib hitstr

- L7 ANSWER 1 OF 1 CAOLD COPYRIGHT 2007 ACS on STN
- AN CA58:5631d CAOLD
- TI 1,5,9-triaminononane derivs.
- AU Ose, Shinsuke; Takamatsu, H.; Saheki, T.
- TI catalytic dehydrogenation of aldehydecollidine AU Oga, Taijiro
- AU Oga, Taijiro IT 96173-74-9 96586-63-9 97573-27-8
- 97573-28-9
- RN 96173-74-9 CAOLD
- CN Benzamide, N-[5-piperidino-1-(4-piperidinobutyl)pentyl]- (7CI) (CA INDEX NAME)

- RN 96586-63-9 CAOLD
- CN Benzamide, N-[5-(1-pyrrolidiny1)-1-[4-(1-pyrrolidiny1)buty1]penty1]- (CA INDEX NAME)

- RN 97573-27-8 CAOLD
- CN Benzamide, N-[5-(3,4-dihydro-2(1H)-isoquinoly1)-1-[4-(3,4-dihydro-2(1H)-isoquinoly1)buty1]penty1]- (7CI) (CA INDEX NAME)

- RN 97573-28-9 CAOLD
- CN Benzamide, N-[5-3,4-dihydro-1(2H)-quinolyl)-1-[4-(3,4-dihydro-1(2H)-quinolyl)butyl]pentyl]- (7CI) (CA INDEX NAME)

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=> s 15 L8 15 L5

=> d 18 1-15 ide

L8 ANSWER 1 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2038939899 CHEMCATS

Catalog Name (CO): ChemDiv Discovery Chemistry Collection Public

Database Publication Date (PD): 2 Oct 2007

Order Number (ON): 6186-3776

(CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-, Chemical Name

2-methyl-2-[(10H-phenothiazin-10-

vlcarbonvl)amino|propvl ester CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

L8 ANSWER 2 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2037170526 CHEMCATS

(CO): New Chemistry Horizons Laboratories Screening Library Catalog Name

Publication Date (PD): 8 Nov 2007

(ON): NCHSC2-79979 Order Number (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-, Chemical Name

2-methyl-2-[(10H-phenothiazin-10-

ylcarbonyl)amino]propyl ester

CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY Structure .

L8 ANSWER 3 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2036468702 CHEMCATS

Catalog Name (CO): Ambinter Stock Screening Collection

Publication Date (PD): 1 Jun 2007

Order Number (ON): AKI-STT-00114311

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,

2-methyl-2-[(10H-phenothiazin-10-

ylcarbonyl)aminolpropyl ester

Synonym (CN): Also sold under Ambinter Order Number(s): STK135578

CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

10/539372

Accession No. (AN): 2036286427 CHEMCATS
Catalog Name (CO): Ambinter Stock Screening Collection
Publication Date (PD): 1 Jun 2007
Chemical Name (CN): Benzamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]CAS Registry No. (RN): 171203-85-3
Supplementary Term (ST): CHEMICAL LIBRARY
Structure :

L8 ANSWER 4 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

L8 ANSWER 5 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN
Accession No. (AN): 203192446 CHEMCATS
Catalog Name (CD): Aurora Screening Library
Publication Date (PD): 6 Sep 2007
Order Number (ON): kbs=008261
Chemical Name (CN): Benzamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]CAS Registry No. Supplementary Term (ST): CHEMICAL LIBRARY
Structure (ST): CHEMICAL LIBRARY

Page 68

$$\begin{array}{c|c} & \text{Ph} & \text{O} \\ & & \parallel \\ & \text{CH-NH-C-Ph} \end{array}$$

L8 ANSWER 6 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2028002259 CHEMCATS

Catalog Name (CO): MicroChemistry Screening Collection

Publication Date (PD): 25 Apr 2007

Order Number (ON): 281369

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,

2-methyl-2-[(10H-phenothiazin-10ylcarbonyl)amino]propyl ester

CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY Structure :

L8 ANSWER 7 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2027695637 CHEMCATS
Catalog Name (CO): Princeton Gold Collection I

Publication Date (PD): 13 Jul 2007

Order Number (ON): OSSK\_540709

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,

2-methyl-2-[(10H-phenothiazin-10ylcarbonyl)amino]propyl ester

CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

L8 ANSWER 8 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2026069766 CHEMCATS Catalog Name (CO): Aurora Screening Library

:

Publication Date (PD): 6 Sep 2007

Order Number (ON): kina-0064310

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-, 2-methyl-2-[(10H-phenothiazin-10-

2-metny1-2-[(10H-phenothiazin-1
ylcarbony1)amino]propyl ester

CAS Registry No. (RN): 511513-88-5 Supplementary Term (ST): CHEMICAL LIBRARY

Structure

10/539372

L8 ANSWER 9 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2023243378 CHEMCATS

(CO): Scientific Exchange Product List Catalog Name

Publication Date

(PD): 18 May 2007 (ON): M-106500 Order Number

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,

2-methyl-2-[(10H-phenothiazin-10vlcarbonyl)amino|propyl ester

CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY

Structure

L8 ANSWER 10 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

(ST): CHEMICAL LIBRARY

Accession No.

(AN): 2021307126 CHEMCATS (CO): AKos Screening Library

Catalog Name Publication Date

Publication Date (PD): 7 Feb 2006 Order Number (ON): AKL-P-1106500

:

Chemical Name

(CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,

2-methyl-2-[(10H-phenothiazin-10ylcarbonyl)amino]propyl ester

Synonym

(CN): Also sold under AKos Order Number(s): STT-00114311,

OWH-2041105 CAS Registry No. (RN): 511513-88-5

Supplementary Term Structure

L8 ANSWER 11 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No.

(AN): 2020286708 CHEMCATS (CO): Interchim Intermediates

Catalog Name Publication Date

e (PD): 9 Jul 2007 (ON): STOCK3S-45083

Order Number (Chemical Name (

(CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,

2-methyl-2-[(10H-phenothiazin-10-ylcarbonyl)amino]propyl ester

Synonym

(CN): Also sold under Interchim Order Number(s):

AJ-292/41685861, STK135578

CAS Registry No. (RN): 511513-88-5 Supplementary Term (ST): CHEMICAL LIBRARY

:

Structure

10/539372

Accession No. (AN): 2020172785 CHEMCATS Catalog Name (CO): Interchim Intermediates Publication Date (PD): 9 Jul 2007 Order Number (ON): STOCK1S-00425 (CN): Benzamide, N-[1-phenyl-5-(1-piperidinyl)pentyl]-Chemical Name CAS Registry No. (RN): 171203-85-3

L8 ANSWER 12 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Supplementary Term (ST): CHEMICAL LIBRARY Structure :

L8 ANSWER 13 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN Accession No. (AN): 2017056336 CHEMCATS

Catalog Name (CO): Compounds For Screening Publication Date (PD): 6 Nov 2007

Order Number (ON): AJ-292/41685861

Chemical Name (CN): 2-methyl-2-[(10H-phenothiazin-10vlcarbonvl)amino]propvl (1,3-dioxooctahydro-2H-

isoindol-2-yl)acetate

(RN): 511513-88-5 CAS Registry No. (ST): CHEMICAL LIBRARY

Supplementary Term Structure :

L8 ANSWER 14 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2014902440 CHEMCATS

(CO): Vitas-M Screening Collection Catalog Name

Publication Date (PD): 7 Jun 2007 Order Number (ON): STK135578

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-,

2-methyl-2-[(10H-phenothiazin-10vlcarbonvl)amino|propvl ester

CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY Structure

## 10/539372

L8 ANSWER 15 OF 15 CHEMCATS COPYRIGHT 2007 ACS on STN

Accession No. (AN): 2010420418 CHEMCATS

Catalog Name (CO): Interbioscreen Compound Library Publication Date (PD): 5 Oct 2007

Order Number (ON): STOCK3S-45083

Chemical Name (CN): 2H-Isoindole-2-acetic acid, octahydro-1,3-dioxo-, 2-methvl-2-[(10H-phenothiazin-10-

ylcarbonyl)amino]propyl ester

CAS Registry No. (RN): 511513-88-5

Supplementary Term (ST): CHEMICAL LIBRARY

Structure :

=> log h COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	30.63	335.70
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-17.16

SESSION WILL BE HELD FOR 120 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 12:17:35 ON 27 DEC 2007